Using in situ data to support satellite ocean color calibration & validation activities

Jeremy Werdell

NASA Goddard Space Flight Center Science Systems & Applications, Inc.

21 January 2010 @ SAC

- 1. in situ data are important for ocean color cal/val
 - vicarious calibration
 - data product validation
 - algorithm development
- 2. lessons learned from maintaining SeaBASS
 - overview & data policies
 - data collection
 - the centralized archive
 - data analysis

- 1. in situ data are important for ocean color cal/val
 - vicarious calibration
 - data product validation
 - algorithm development

overview
operational / MOBY
model-based
alternative data sources
population statistics

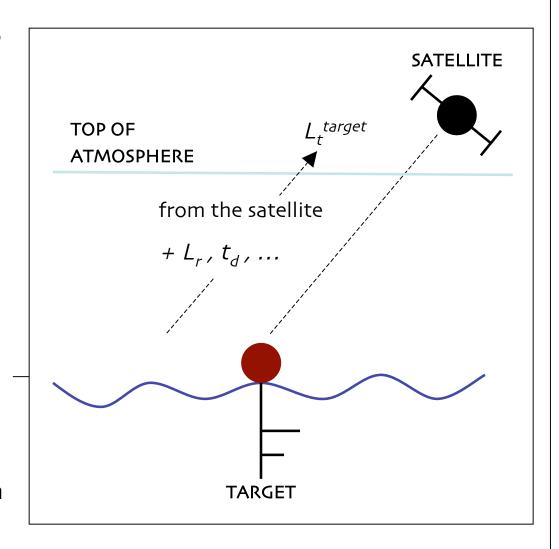
- 2. lessons learned from maintaining SeaBASS
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vicarious calibration

what is vicarious calibration?

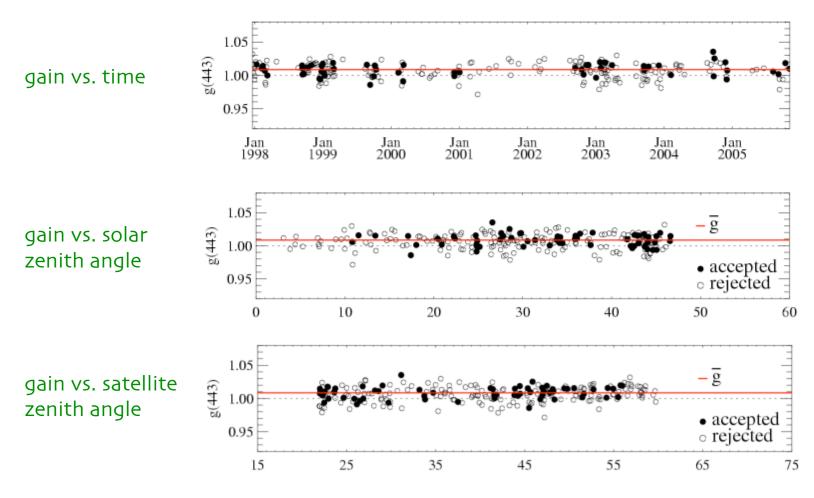
spectral on-orbit calibrations

- 1. instrument calibration
 - e.g., focal plane temperature
- 2. temporal calibration
 - reference Sun or Moon
- 3. absolute (vicarious) calibration
 - reference Earth surface
 - final, single gain adjustment
 - calibration of the combined instrument + algorithm system



vicarious calibration

a single, spectral radiometric adjustment

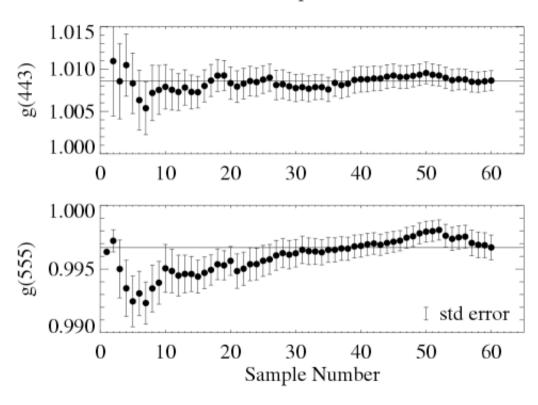


B.A. Franz, S.W. Bailey, P.J. Werdell, and C.R. McClain, "Sensor-independent approach to the vicarious calibration of satellite ocean color radiometry," Applied Optics 46, 5068-5082 (2007).

vicarious calibration

2-3 years to achieve stable vicarious calibration

Gain Vs. Sample Size



B.A. Franz, S.W. Bailey, P.J. Werdell, and C.R. McClain, "Sensor-independent approach to the vicarious calibration of satellite ocean color radiometry," Applied Optics 46, 5068-5082 (2007).

operational vicarious calibration

MOBY - the Marine Optical BuoY

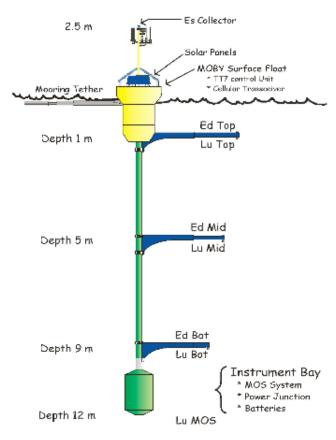


Fig. 1. Schematic diagram of MOBY.

maintained by NOAA & Moss Landing Marine Laboratory

20 miles west of Lanai, Hawaii

 $L_u(\lambda)$ and $E_d(\lambda)$ at nominal depths of 1, 5, and 9 meters, plus $E_s(\lambda)$

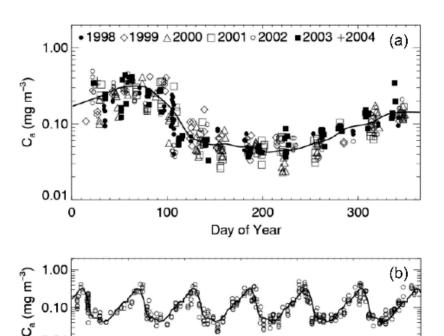
spectral range is 340-955 nm & spectral resolution is 0.6 nm

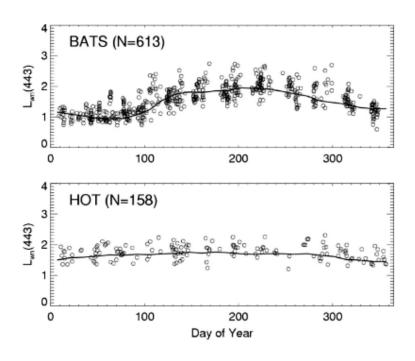
hyperspectral data convolved to specific bandpasses of each satellite

approximately 450-700 samples per year for MODIS-Aqua

model-based vicarious calibration

build a climatology using a longterm chlorophyll-a record (this is for BATS, near Bermuda) ...





... then, develop a radiometric climatology using an ocean reflectance model (e.g., Morel and Maritorena 2001)

P.J. Werdell, S.W. Bailey, B.A. Franz, A. Morel, and C.R. McClain, "On-orbit vicarious calibration of ocean color sensors using an ocean surface reflectance model," Applied Optics 46, 5649-5666 (2007).

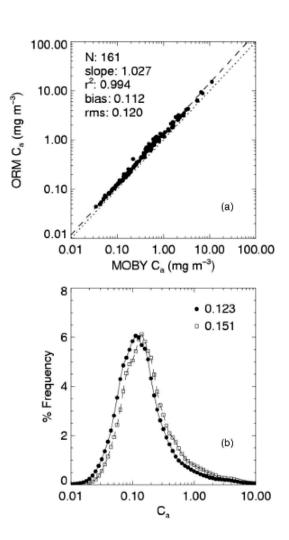
model-based vicarious calibration

Table 3. Percent Differences a Between the MOBY and ORM \bar{g}

	412	443	490	510	555	670
BATS	-0.31	-1.18	-1.14	-0.52	0.14	-0.07
HOTS	-0.74	-0.53	-0.48	-0.14	0.44	-0.21
BATS + HOTS	-0.52	-0.86	-0.81	-0.33	0.29	-0.13

^aCalculated using $(\bar{g}_{ORM} - \bar{g}_{MOBY}) \times 100\%/\bar{g}_{MOBY}$.

model-based gains typically differ from MOBY gains by < 1%



P.J. Werdell, S.W. Bailey, B.A. Franz, A. Morel, and C.R. McClain, "On-orbit vicarious calibration of ocean color sensors using an ocean surface reflectance model," Applied Optics 46, 5649-5666 (2007).

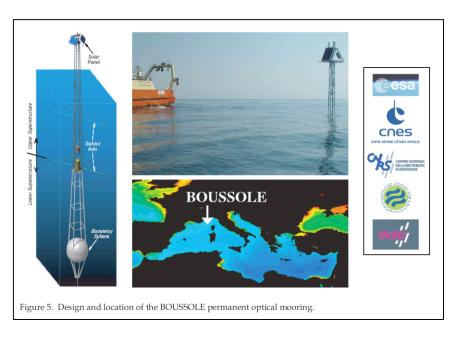
alternative in situ data for vicarious calibration

in situ data from other sources, such as global ship-based data sets (NOMAD), alternate buoys (BOUSSOLE), or networks of above water sensors (AERONET-OC)

AERONET-OC

Figure 3. Clockwise from left a SeaPRISM in operation; locations of the network testing phase AERONET-OC stations (2001 - 2005; see http://aeronot.gsfc.nasa.gov for acronym definitions and an updated list of SeaPRISM stations); and, a detailed view of the location of the AAOT.

BOUSSOLE



S.W. Bailey, S.B. Hooker D. Antoine, B.A. Franz, and P.J. Werdell, "Sources and assumptions for the vicarious calibration of ocean color satellite observations," Applied Optics 47, 4186-4203 (2008).

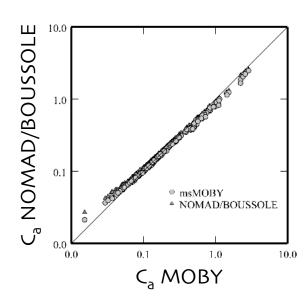
alternative in situ data for vicarious calibration

Table 2. Vicarious Gain Coefficients for Standard Method^a

Source	N	412	443	490	510	555	670
MOBY	166	1.0368	1.0132	0.9918	0.9982	0.9993	0.9729
(σ)		(0.009)	(0.009)	(0.008)	(0.009)	(0.009)	(0.007)
CV		1.736	1.777	1.613	1.803	1.801	1.439
NOMAD	64	1.0395	1.0135	0.9967	0.9962	0.9989	0.9693
(σ)		(0.013)	(0.013)	(0.014)	(0.017)	(0.013)	(0.009)
UPD		0.1300	0.01480	0.2464	-0.1003	-0.0200	-0.1854
$BOUSSOLE^b$	46	1.0402^{c}	1.0129	0.9961	1.0015	1.0007	0.9672
(σ)		(0.005)	(0.027)	(0.033)	(0.031)	(0.021)	(0.006)
UPD		0.1637	-0.0148	0.2163	0.1650	0.0700	-0.2938

^aGain coefficients using the threshold criteria defined in [4]. The standard deviations are shown in parentheses. bC_a threshold increased to 0.25 mg m⁻³ for the BOUSSOLE data set to bring the N to a minimum of 40. The 412 nm data for BOUSSOLE used only 9 points.

gains calculated using alternative *in situ* data typically differ from MOBY by < 0.3%

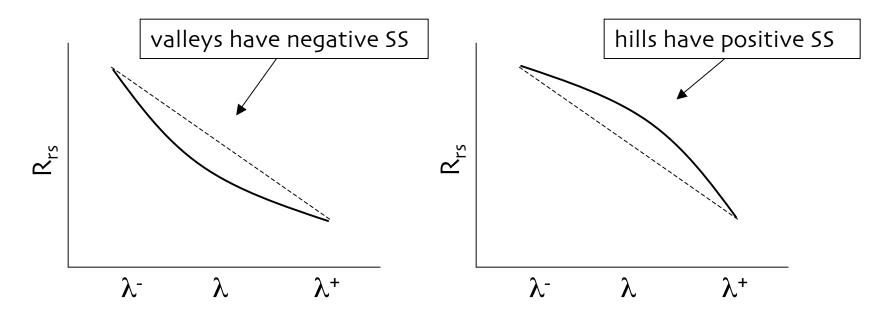


S.W. Bailey, S.B. Hooker D. Antoine, B.A. Franz, and P.J. Werdell, "Sources and assumptions for the vicarious calibration of ocean color satellite observations," Applied Optics 47, 4186-4203 (2008).

tuning vicarious calibration using population statistics

compare spectral shapes of in situ & satellite populations

$$SS(\lambda) = R_{rs}(\lambda) - R_{rs}(\lambda^{-}) - \left[R_{rs}(\lambda^{+}) - R_{rs}(\lambda^{-})\right] \left(\frac{\lambda - \lambda^{-}}{\lambda^{+} - \lambda^{-}}\right)$$

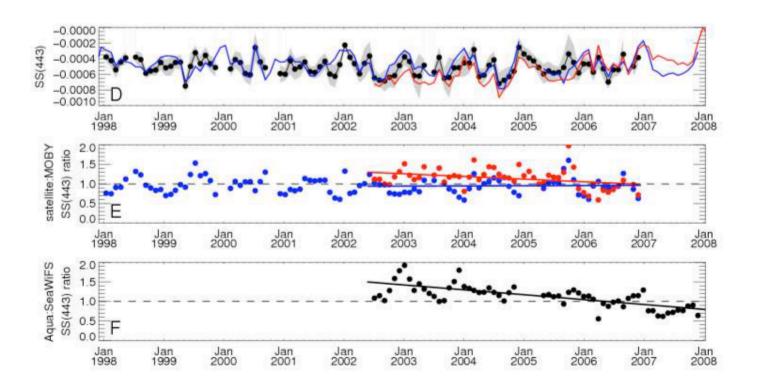


spectral shape @ 443 nm, SS(443), uses R_{rs} (412), R_{rs} (443), & R_{rs} (490)

R.P. Stumpf and P.J. Werdell, "Adjustment of ocean color sensor calibration through multi-band statistics," Optics Express 18, 401-412 (2010)

tuning vicarious calibration using population statistics

in situ, SeaWiFS, & MODIS-Aqua spectral shapes compared at MOBY site



R.P. Stumpf and P.J. Werdell, "Adjustment of ocean color sensor calibration through multi-band statistics," Optics Express 18, 401-412 (2010)

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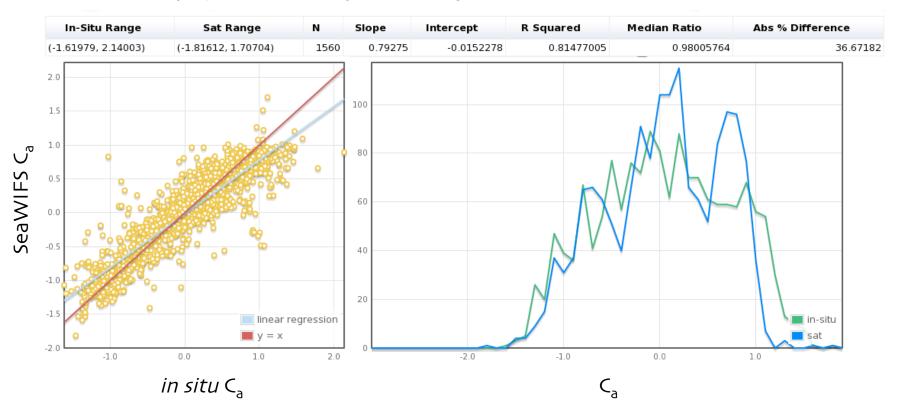
Level-2 match-ups Level-2 time-series community efforts

- 2. lessons learned from maintaining SeaBASS
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Level-2 match-ups

comparison of "coincident" in situ & satellite measurements

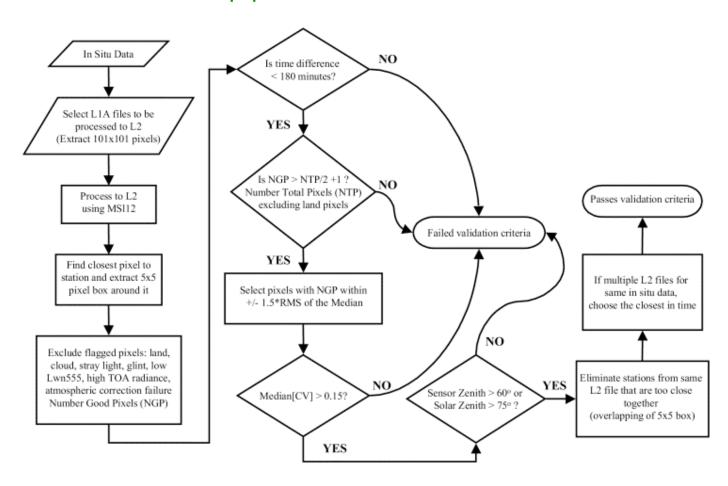
SeaWiFS chlorophyll-a match-ups (OC4 algorithm):



S.W. Bailey and P.J. Werdell, "A multi-sensor approach for the on-orbit validation of ocean color satellite data products," Remote Sensing of Environment 102, 12-23 (2006)

Level-2 match-ups

general flow of match-up process, with exclusion criteria



S.W. Bailey and P.J. Werdell, "A multi-sensor approach for the on-orbit validation of ocean color satellite data products," Remote Sensing of Environment 102, 12-23 (2006)

PJW, NASA/SSAI, 21 Jan 2010 @ SAC

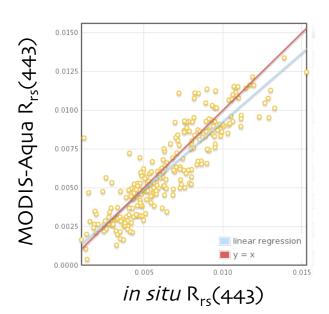
Level-2 match-ups

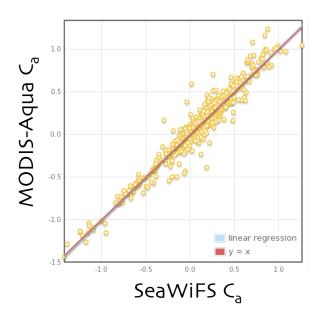
results publicly posted online at:

http://seabass.gsfc.nasa.gov/seabasscgi/validation_search.cgi

highlights

- analyze match-ups for satellite-to-in situ & satellite-to-satellite
- search by date, location, water depth, or specific cruise
- customize exclusion criteria
- all operational data products



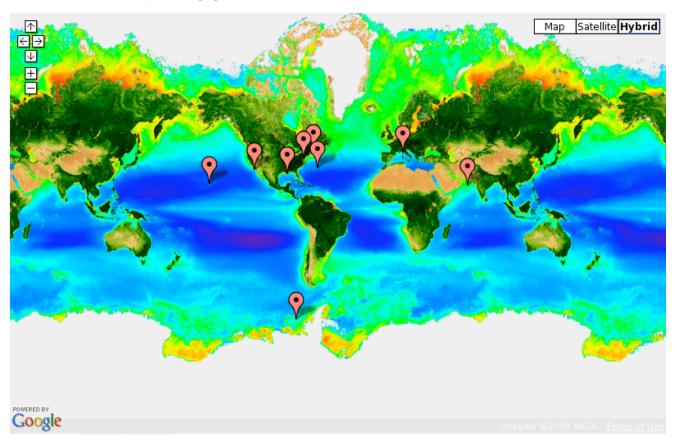


S.W. Bailey and P.J. Werdell, "A multi-sensor approach for the on-orbit validation of ocean color satellite data products," Remote Sensing of Environment 102, 12-23 (2006)

Level-2 time-series analyses

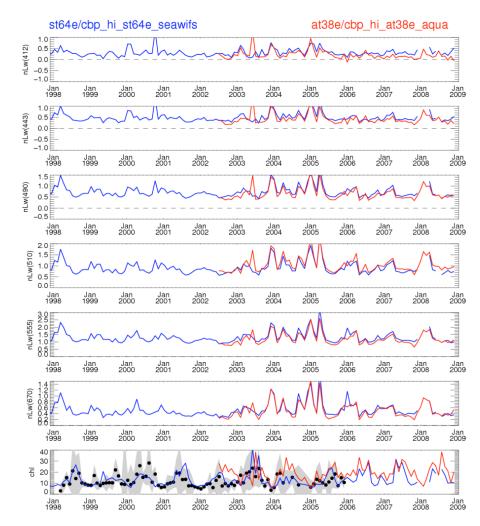
results publicly posted online at: http://oceancolor.gsfc.nasa.gov/cgi/regions.cgi

9 regions currently supported



P.J. Werdell, S.W. Bailey, L.W. Harding Jr., Gene C. Feldman, and C.R. McClain, "Regional and seasonal variability of chorophyll-a in Chesapeake Bay as observed by SeaWiFS and MODIS-Aqua," Remote Sensing of Environment 113, 1319-1330 (2009).

Level-2 time-series analyses

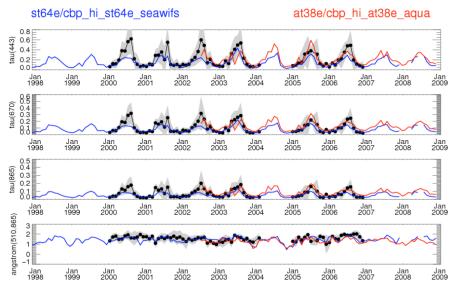


monthly time-series

SeaWiFS vs. MODIS-Aqua vs. in situ

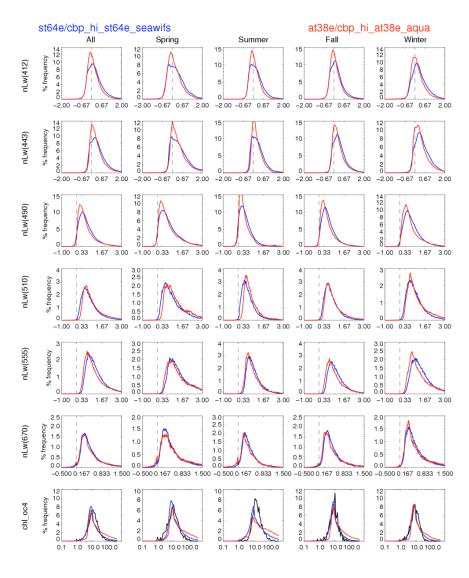
upper third of Chesapeake Bay

in situ data from Chesapeake Bay Program (C_a) & AERONET (AOTs)



P.J. Werdell, S.W. Bailey, L.W. Harding Jr., Gene C. Feldman, and C.R. McClain, "Regional and seasonal variability of chorophyll-a in Chesapeake Bay as observed by SeaWiFS and MODIS-Aqua," Remote Sensing of Environment 113, 1319-1330 (2009).

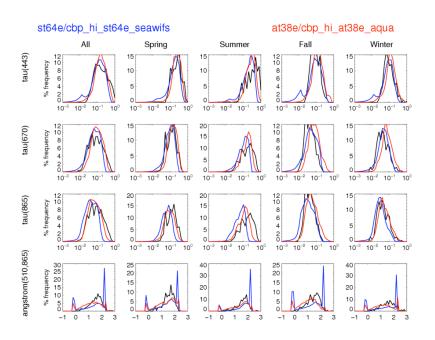
Level-2 time-series analyses



seasonal frequency distributions SeaWiFS vs. MODIS-Aqua vs. in situ

upper third of Chesapeake Bay

in situ data from Chesapeake Bay Program (C_a) & AERONET (AOTs)



P.J. Werdell, S.W. Bailey, L.W. Harding Jr., Gene C. Feldman, and C.R. McClain, "Regional and seasonal variability of chorophyll-a in Chesapeake Bay as observed by SeaWiFS and MODIS-Aqua," Remote Sensing of Environment 113, 1319-1330 (2009).



ISI Web of Science search for "ocean color validation" yields 299 results

result #2 (as of 7 Jan 2010): K.N. Babu, A.K. Shukla, G.P. Matondkar, S.K. Singh, S. Sawant, "Characterization of chlorophyll-a over CAL-VAL site at Kavaratti in the Lakshadweep Sea," Marine Geodesy 32, 345-354 (2009)

OBPG "match-up" Remote Sensing of Environment paper cited ~ 45 times

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NOMAD
operational algorithms
generic IOP algorithm
atmospheric correction
community efforts

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NOMAD ~ NASA bio-Optical Marine Algorithm Dataset

SeaBASS consists of original files from data collectors

radiometry, spectroscopy, pigments, and CTD all in separate files most data are depth-resolved, i.e., no surface (o-) values! lots of replicate data

realizing the difficulty in using these data for algorithm development, the OBPG

evaluated all SeaBASS radiometry, spectroscopy, pigments, and CTD estimated surface (o-) values from these data (used for validation!) identified coincident observations generated a consolidated, merged data set

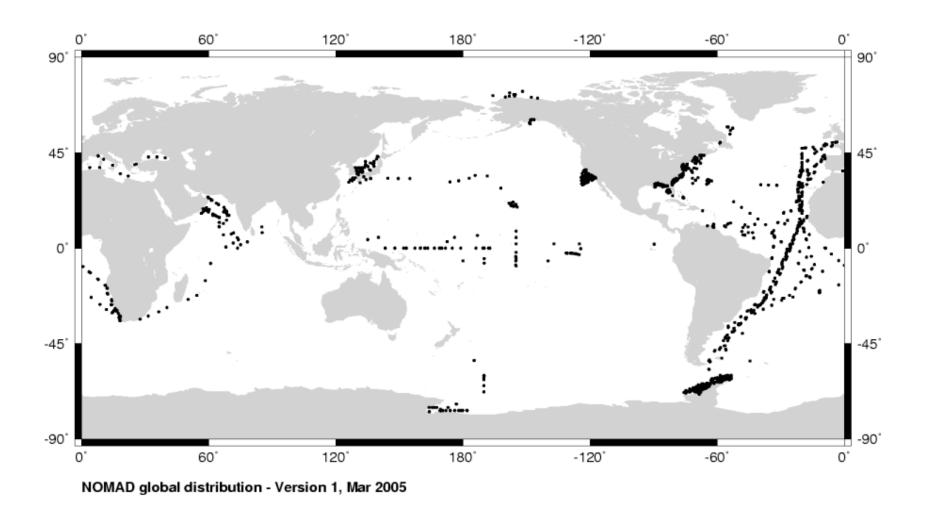
NOMAD is fully publicly available, as are its source data within SeaBASS

3,467 coincident observations of $L_w(\lambda)$, $E_s(\lambda)$, $K_d(\lambda)$, & C_a Wt, Sal, $b_b(\lambda)$, and $a(\lambda)$ where available metadata includes date, location, & cruise name plus, NCDC OISST, NGDC ETOPO2, & processing flags

P.J. Werdell and S.W. Bailey, "An improved in-situ bio-optical data set for ocean color algorithm development and satellite data product validation," Remote Sensing of Environment 98, 122-140 (2005)

PJW, NASA/SSAI, 21 Jan 2010 @ SAC

NOMAD ~ NASA bio-Optical Marine Algorithm Dataset



P.J. Werdell and S.W. Bailey, "An improved in-situ bio-optical data set for ocean color algorithm development and satellite data product validation," Remote Sensing of Environment 98, 122-140 (2005)

operational empirical algorithms

operational empirical (statistical) algorithms typically have a form that resembles

$$log_{10}(C_{a}) = c_{0} + \sum_{i=1}^{N} c_{i}log_{10} \left(\frac{R_{rs}(\lambda_{b})}{R_{rs}(\lambda_{g})} \right)$$

including all OC* & KD* algorithms developed by the OBPG, plus POC, TSM, etc. algorithms developed elsewhere

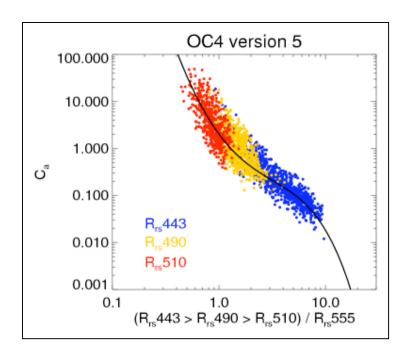


Table 1Coefficients for the OC version 5 algorithms (O'Reilly, personal communication).

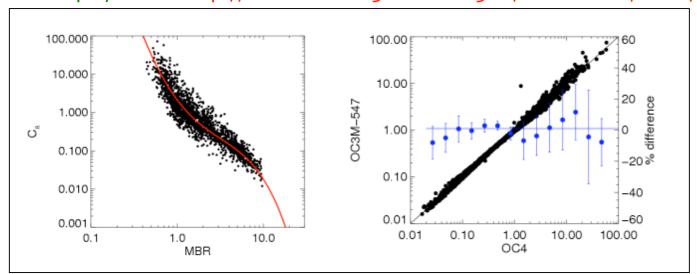
	λ_{b}	λ_{g}	C ₀	c ₁	<i>c</i> ₂	C ₃	C4
OC4	443,490,510	555	0.3080	-3.0882	3.0440	- 1.2013	-0.7992
OC3S ^a	443,490	555	0.2409	-2.4768	1.5296	0.1061	-1.1077
OC3M _p	443,488	551	0.2254	-2.6354	1.8071	0.0063	-1.2931

a For SeaWiFS.

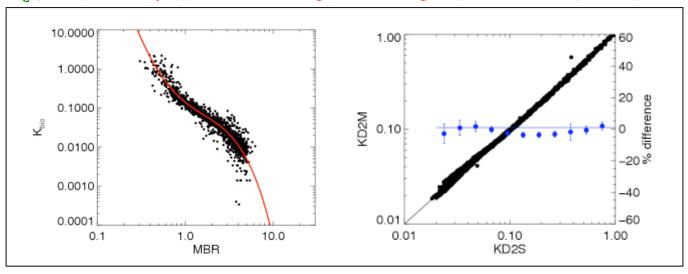
b For MODIS-Aqua.

operational empirical algorithms

chlorophyll-a ~ http://oceancolor.gsfc.nasa.gov/ANALYSIS/ocv6/



K_d(490) ~ http://oceancolor.gsfc.nasa.gov/ANALYSIS/kdv4/



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the Generic IOP model (GIOP)

construction (& deconstruction) of an semi-analytic algorithm ...

$$R_{rs} \approx func \left(\frac{b_b}{a + b_b} \right)$$

 $R_{rs} \approx func\left(\frac{b_b}{a+b_c}\right)$ satellite provides $R_{rs}(\lambda)$ and $b_b(\lambda)$ are desired products

Spectral Optimization:

- * define shape functions for (e.g.) $b_{bp}(\lambda)$, $a_{dq}(\lambda)$, $a_{ph}(\lambda)$
- * solution via L-M, matrix inversion, etc.
- * ex: RP95, HL96, GSM

Bulk Inversion:

- * no predefined shapes
- * piece-wise solution: $b_{bp}(\lambda)$, then $a(\lambda)$, via (empirical) $K_d(\lambda)$ via RTE
- * ex: LSoo

Spectral Deconvolution:

- * partially define shape functions for $p^{pp}(y), q^{qq}(y)$
- * piece-wise solution: $b_{bp}(\lambda)$, then $a(\lambda)$, then $a_{dq}(\lambda) + a_{ph}(\lambda)$
- * ex: QAA, PML, NIWA

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the Generic IOP model (GIOP)

specify sensor wavelengths to fit

e.g., 412,443,490,510,555

select a_{ph} form and set params

tabulated: λ , $a_{ph}^*(\lambda)$

dynamic: Bricaud, Ciotti, Lee

select a_{da} form and set params

exponential: λ_o , S

dynamic: QAA, OBPG

select b_{bp} form and set params

power law: λ_o , η

dynamic: QAA, LSoo, Ciotti, Morel

select $r_{rs}[o-]$ to $b_b/(a+b_b)$

quadratic

f/Q: Morel (tbd: PML, Lee)

specify inversion method

Levenburg-Marquardt

Amoeba (downhill simplex)

Lower-Upper Decomposition

Singular-Value Decomposition

specify output products

 $a(\lambda)$, $a_{ph}(\lambda)$, $a_{dq}(\lambda)$, $b_b(\lambda)$, $b_{bp}(\lambda)$

 λ = any sensor wavelength(s)

 C_a (given a_{ph} * at λ_o)

 η , S (dynamic model params)

internal flags

http://oceancolor.gsfc.nasa.gov/MEETINGS/OOXIX/IOP/

atmospheric correction

in situ data ... it's not just for in-water algorithm development anymore

- development of new aerosol tables (via AERONET)

Z. Ahmad, B.A. Franz, C.R. McClain, E.J. Kwiatkowska, P.J. Werdell, E. Shettle, and B.N Holben, "Aerosol models for the retrieval of aerosol optical thickness and normalized water-leaving radiances from the SeaWiFS and MODIS sensors over coastal regions and open oceans," to be submitted to Applied Optics

- refinement of the correction for non-zero $R_{rs}(NIR)$

S.W. Bailey, B.A. Franz, P.J. Werdell, "Estimation of near-infrared water-leaving reflectance for satellite ocean color data processing," submitted to Optics Express

- refinement of the correction bidirectional effects (f/Q)
- evaluation of the correction for spectral bandpass effects

community algorithm development efforts

International Ocean Color Coordinating Group (IOCCG)

- working group "Ocean-Colour Algorithms" (Report 5)
- working group "Phytoplankton Functional Types"
- proposed working group "Regional bio-Optical algorithms Initiative (ROI)"

Optical Water Type classification

T.S. Moore, J.W. Campbell, and M.D. Dowell, "A class-based approach to characterizing and mapping the uncertainty of the MODIS ocean chlorophyll product," Remote Sensing of Environment 113, 2424-2430 (2009)

how to summarize the 100's of other bio-optical algorithm development papers?

NOMAD Remote Sensing of Environment paper cited ~ 40 times

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philosophy & data policies

the SeaWiFS Bio-optical Archive & Storage System (SeaBASS)

archive for bio-optical data & related oceanographic / atmospheric measurements

data contributed by research groups from ~50 institutions in 15 countries

50,000 data files from over 2,000 field campaigns, as of January 2010, including:

- 40,000 radiometric (AOP) stations
- 70,000 pigment (CHL) stations
- 25,000 spectroscopy (IOP) stations
- 17,000 aerosol optical thickness (AOT) stations

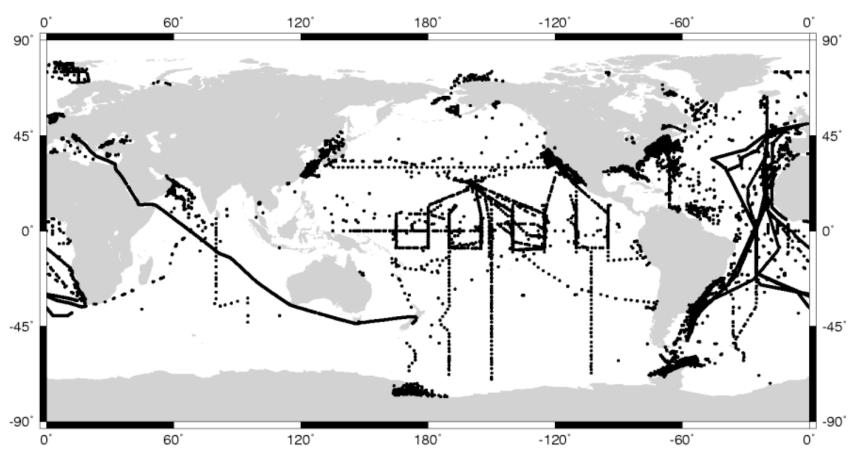
all data are accessible online:

- publicly available via SeaBASS Web site
- periodically released to National Oceanographic Data Center

http://seabass.gsfc.nasa.gov

P.J. Werdell and S.W. Bailey, "The SeaWiFS Bio-optical Archive and Storage System (SeaBASS): Current architecture and implementation," NASA/TM-2002-211617, NASA Goddard Space Flight Center, 45 pp. (2002).

philosophy & data policies



SeaBASS AOPs, IOPs, and Chl, Jan 2008

philosophy & data policies

data submission policy

- permanent archive for NASA Ocean Biology & Biogeochemistry (OB&B) data
- data submitted to archive within 1-year of date of collection (DOC)
- periodic release to NOAA National Oceanographic Data Center
- planned periodic release to WHOI BCO-DMO

data access policy

- follows NASA Earth Science Data & Information Policy
- all data publicly available for research and education use
- original contributors to be offered authorship for 3-years of DOC
- contributors, NASA, & SeaBASS always to be acknowledged

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data collection

all data to be collected (whenever possible) following community-vetted protocols prescribed in NASA Technical Memoranda Series (6 Volumes)

- Ocean Optics Protocols for Ocean Color Sensor Validation
- http://oceancolor.gsfc.nasa.gov/DOCS/TechMemo/

all OB&B funded high performance liquid chromotography (HPLC) samples processed by Horn Point Laboratory @ the University of Maryland

organization & participation in international data collection & processing round robins & workshops (e.g., SeaHARRE & SIRREX)

NASA Calibration & Validation Office (CVO)

- participation in field campaigns
- instrument development
- refinement of data collection & processing protocols
- organization of instrument round

"complete" data sets ~ validation vs. algorithm development vs. science

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benefits of a centralized archive

consolidated ...

- data acquisition by community members
- file formats
- quality control & quality assurance
- permanent (redudant) archival

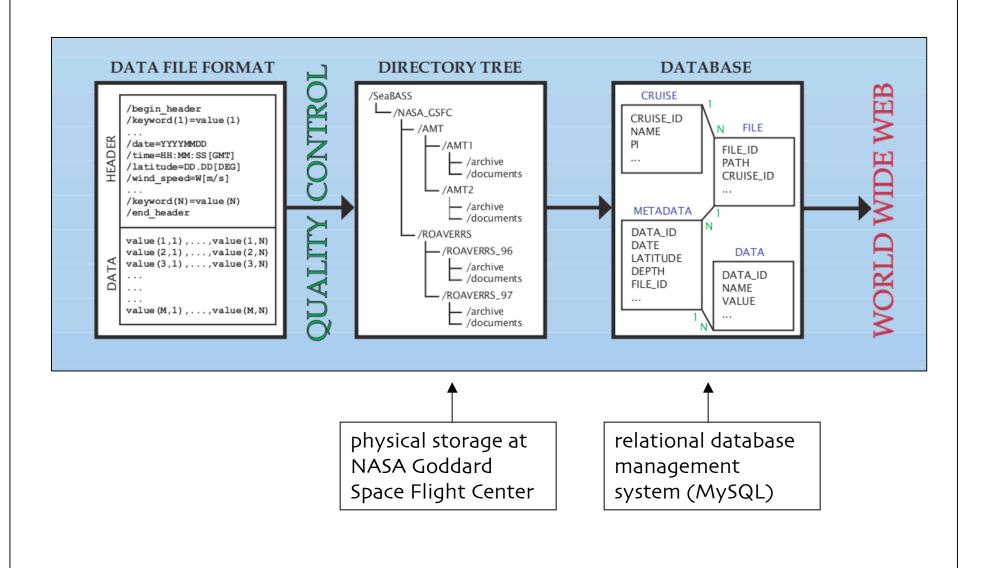
facilitates ...

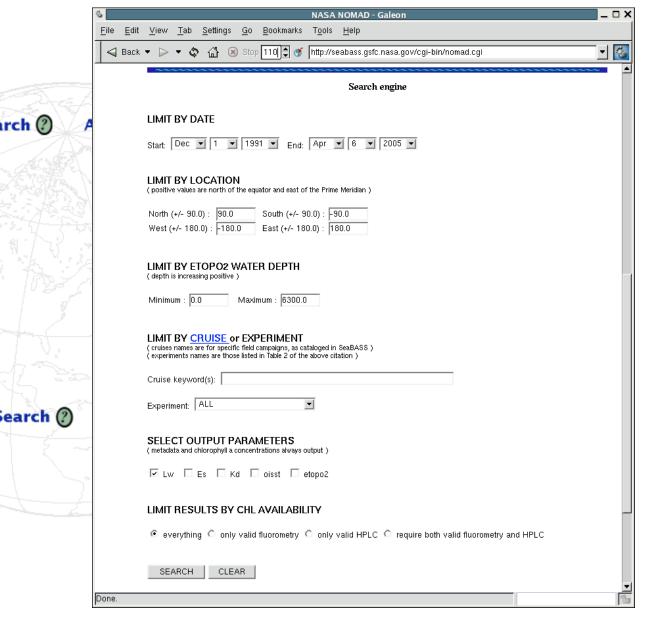
- systematic post-processing
- rigorous quality control & quality assurance
- development of algorithm development & validation data sets
- centralized cal/val activities

SeaBASS file format: - ASCII text for platform independence

- matrix of data preceded by predefined metadata headers

```
/begin header
/investigators=John Smith, Mary Johnson
/affiliations-State University
                                                           /begin header<cr>
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/wind speed=5.0
/wave height=1.0
  COMMENTS
  Slightly overcast, with large cumulous on horizon. Wind from NE.
  Turner fluorometer last calibrated: 12 December 2000
/missing=-999
<u>/deliniter</u>=tab
/fields=time, depth, CHL, PHAEO, Tpg
/units=hh:nm:ss,m,ng/m^3,ng/m^3,ng/n^3
/end header
16:0T:30
                         2.355 0.785
16:03:45
                         2.180 1.005
                                        PJW, NASA/SSAI, 21 Jan 2010 @ SAC
```





Bio-optical Search (?)

Pigment Locator (?)

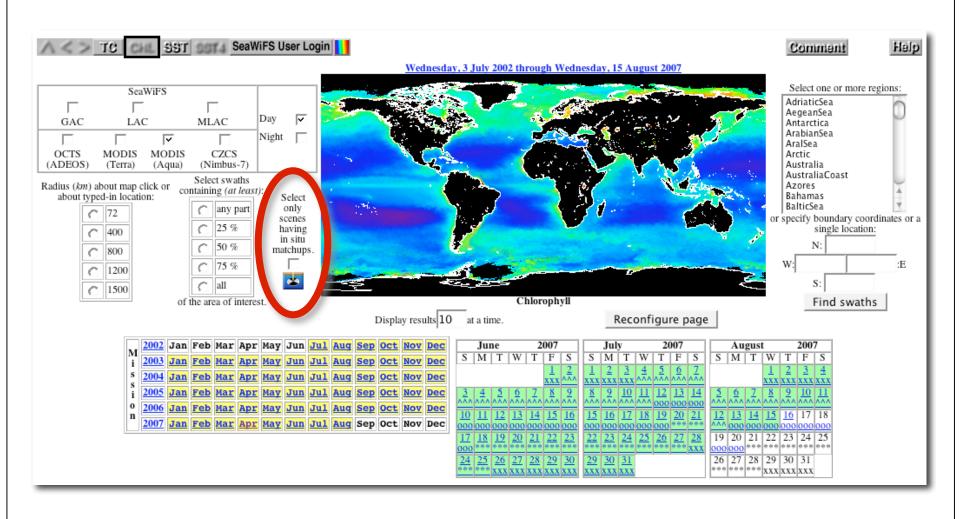
Aerosol Locator ②

General Search 🕖

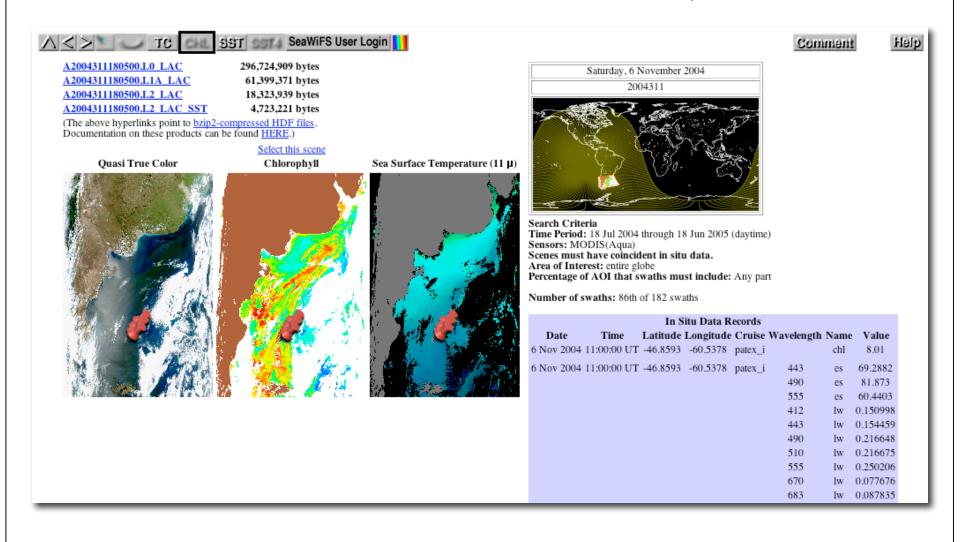
Cruise Search (2)

Validation Cruise Search (2)

NOMAD & validation data are available via the OBPG Level 1/2 Browser



NOMAD & validation data are available via the OBPG Level 1/2 Browser



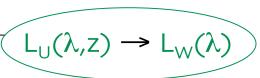
- 1. in situ data are important for ocean color cal/val
 - vicarious calibration
 - data product validation
 - algorithm development
- 2. lessons learned from maintaining SeaBASS
 - overview & data policies
 - data collection
 - the centralized archive
 - data analysis

SeaBASS

AOP(λ ,z), IOP(λ ,z), & C_a/CTD/bottle(z)

format provided by PI

minimal exclusion



VDS (Validation Data Set)

AOP(λ ,o⁺), IOP(λ , o⁺), & C_a/CTD/bottle(o⁺)

no restrictions on coincidence

exclusion criteria applied (x2) / data reduction

calibration quality with protocol adherence

NOMAD

 \rightarrow AOP(λ ,o⁺) + IOP(λ , o⁺) + C_a/CTD/bottle(o⁺)

coincidence requirement

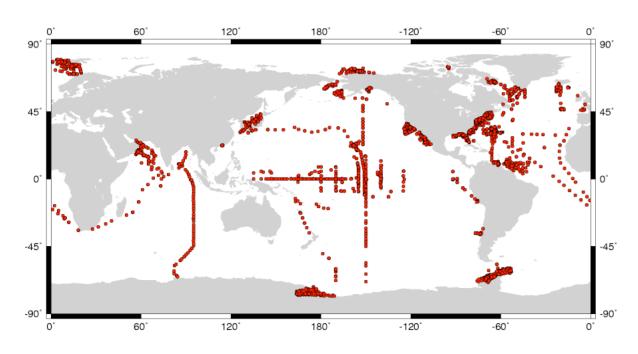
PJW, NASA/SSAI, 21 Jan 2010 @ SAC

data analysis

SeaBASS includes ~12,000 AOP depth profiles ...

... collected on ~850 field campaigns ...

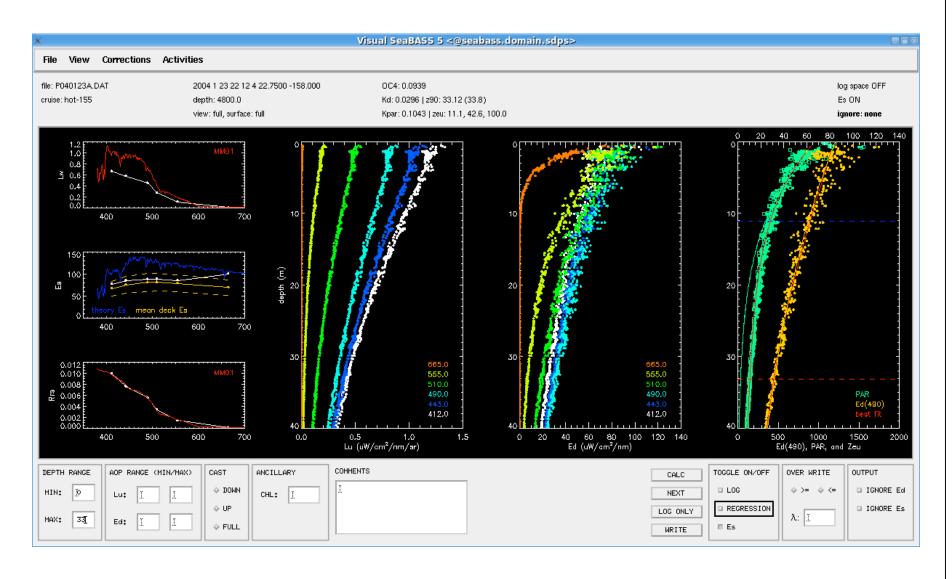
... by ~30 different PIs & a variety of instruments

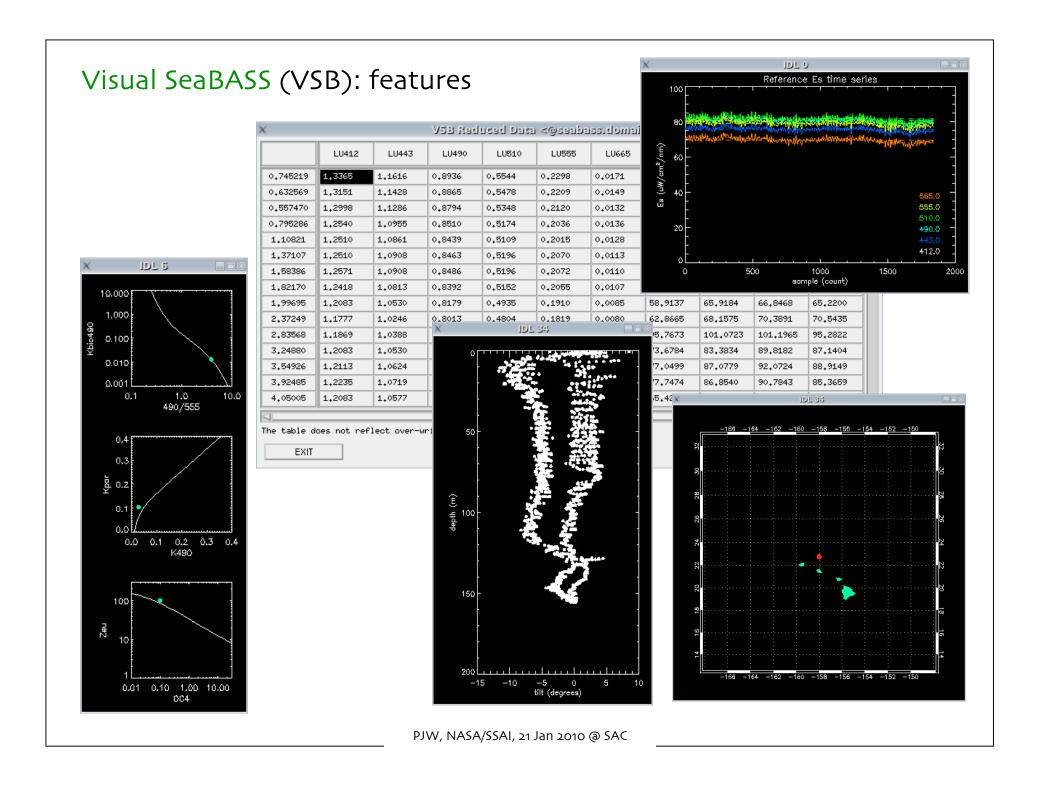


want generic post-processor to minimize PI / instrument differences

data analysis

Visual SeaBASS (VSB): main window





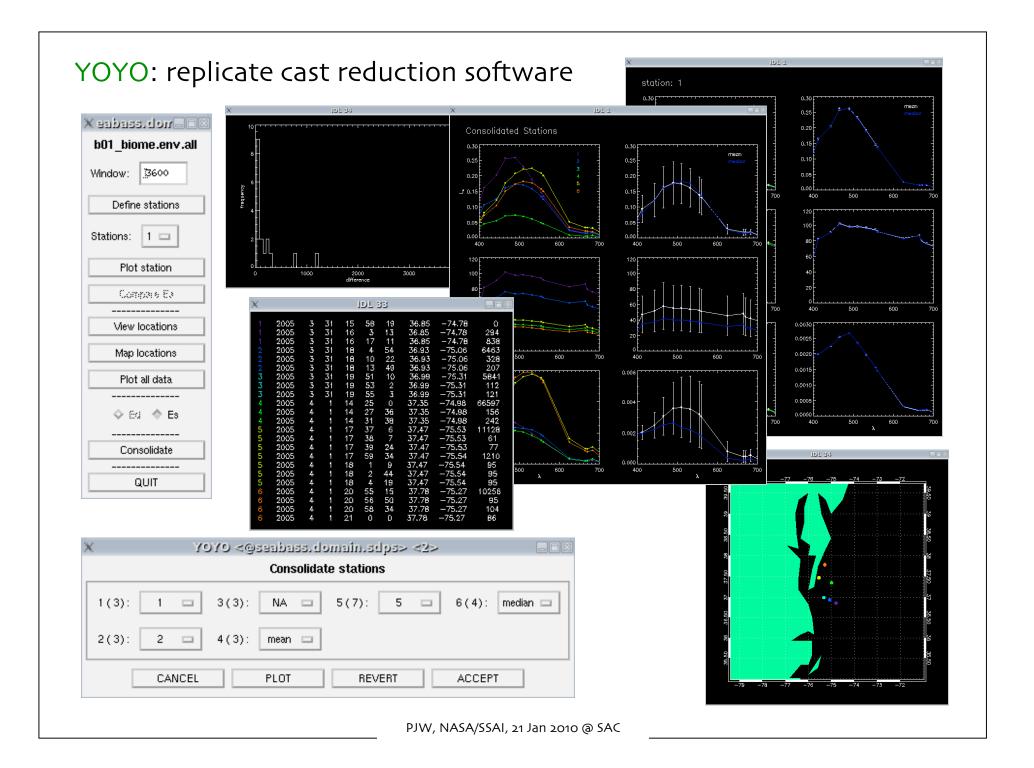
data analysis

calculate & report:

$$\begin{split} & L_W(\lambda) \\ & E_D(o^+,\lambda), \, E_S(\lambda) \\ & K_D(\lambda), \, z_{90}(\lambda) \, \big[\, \text{Mueller 2000; } E_D(z_{90}) = E_D(o^-) \, e^{-1} \, \big] \\ & K_{PAR}, \, z_{PAR}(37,10,1\%) \, \big[\, \text{Morel et al. 2007} \, \big] \\ & \text{regression statistics } \big[\, \text{incl. near-surface } K_D(\lambda) \, \& \, K_{LU}(\lambda) \, \big] \\ & \text{processing flags} \end{split}$$

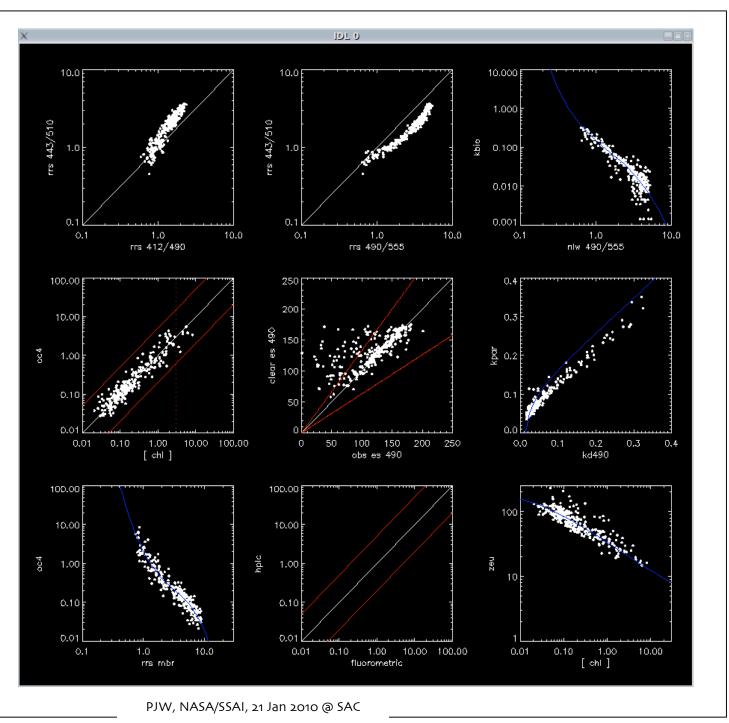
processing notes, extrapolation intervals, & statistics logged output written to SeaBASS-style file (usually 1 file per cruise)

~30% (± 20%) data files fail various exclusion criteria [TBD] replicates remain & are addressed elsewhere



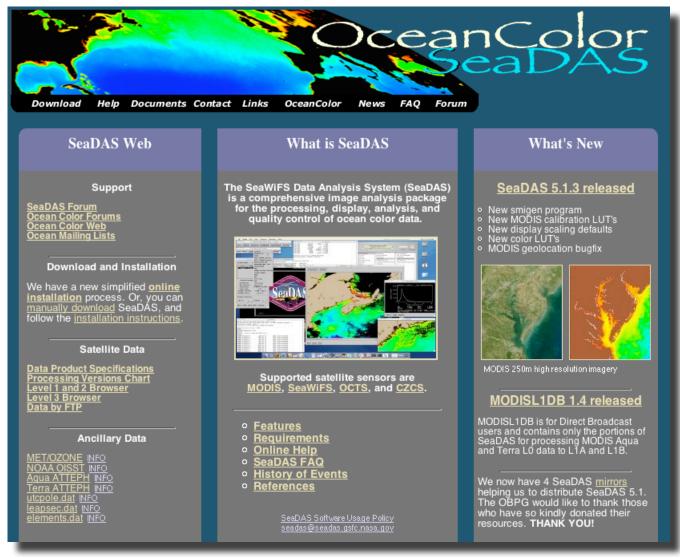
evaluation at the cruise level:

AMT 1 - 8



SeaDAS

many of these capabilities will be included in future releases of the SeaWiFS Data Analysis System (SeaDAS)



PJW, NASA/SSAI, 21 Jan 2010 @ SAC

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vicarious calibration

why do we need a vicarious calibration?

because uncertainties remain after direct calibration

MODIS absolute radiometric accuracy

reflective solar bands (0.41–2.1 μ m): \pm 2% in reflectance and \pm 5% in radiance

MODIS relative accuracy over time

reflective solar bands (0.41–2.1 μ m): \pm 0.2% in reflectance

alternative in situ data for vicarious calibration

preliminary analysis using alternative *in situ* data sources for vicarious calibration

	n	412	443	490	510	555	670
MOBY	32	1.0360	1.0126	0.9910	0.9956	0.9939	0.9627
SSRM	28	1.0395 (0.34)	1.0108 (-0.18)	0.9883 (-0.27)	0.9864 (-0.92)	0.9907 (-0.32)	0.9659 (0.33)
SeaPRISM	8	1.0487 (1.23)	1.0163 (0.37)	1.0013 (1.04)	1.0198 (2.43)	1.0068 (1.30)	0.9838 (2.19)
BOUSSOLE	18	1.0008 (-3.40)	1.0149 (0.23)	0.9968 (0.59)	1.0010 (0.54)	0.9998 (0.59)	0.9623 (-0.04)

Table 2. SeaWiFS vicarious gains for MOBY and the three alternate L_{wn} sources. Relative differences (%) in parentheses. Gains with the lowest absolute differences are **highlighted in red**. For SeaPRISM, g(490) and g(510) were calculated using $L_{wn}(501)$, which impacts its C_a validation results in Figure 4.

S.W. Bailey, S.B. Hooker D. Antoine, B.A. Franz, and P.J. Werdell, "Sources and assumptions for the vicarious calibration of ocean color satellite observations," Applied Optics 47, 4186-4203 (2008).